Quantum-Classical System: Simple Harmonic Oscillator

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Abstract

Problems concerning with application of quantum rules on classical phenomena have been widely studied, for which lifted up the idea about quantization and uncertainty principle. Energy quantization on classical example of simple harmonic oscillator has been reviewed in this paper.

1 Introduction

In the past few years applications of quantum rules on many classical problems have been widely studied, both theoretically and experimentally[1-3]. Such applications lifted up problems concerning with quantization and the uncertainty principle, which are not considered in the classical scheme. These treatments are of considerable importance these days owing to their prospective applications or even more establish a new field, for example, in quantum computation and quantum cryptography[4-6].

How can we realize classical problems in quantum scheme? Let us consider a simple one-dimensional classical harmonic oscillator of mass m with kinetic energy $p^2/2m$ and potential energy $kq^2/2 = m\omega^2 q^2/2$, where k is a constant. Thus, it leads to the corresponding Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2}kq^2 \qquad \ldots(1).$$

This describes a force $-kq$, for which Newton's second law

$$m\frac{d^2q}{dt^2} = -kx \qquad \ldots(2).$$

has oscillating solutions $A\sin(\omega t) + B\cos(\omega t)$, with $\omega = (k/m)^{1/2}$ being the angular frequency of vibration, which allow us to rewrite the Hamiltonian into the form

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2}m\omega^2 q^2 \qquad \ldots(3).$$

In the quantum case we introduce the equation

$$-\frac{\hbar^2}{2m}\frac{d^2u(q)}{dq^2} + V(q)u(q) = Eu(q) \qquad \ldots(4).$$

Equation (4) known as time-independent Schrödinger equation and the solutions $u(q)$ are called wave function which always take the form

$$\psi(q,t) = u(q)\exp(-iEt/\hbar) \qquad \ldots(5).$$

2 Quantum Simple Harmonic Oscillator

2.1 The energy quantization

Let us use the quantum theory to the simple one-dimensional classical harmonic oscillator we have introduced above. In the quantum case we substitute the potential energy equation $kq^2/2$ into Eq. (4) to obtain

$$\frac{d^2u}{dz^2} + (2\epsilon - z^2)u = 0 \qquad \ldots(6).$$

where

$$z = (\frac{m\omega}{\hbar})^{1/2}q \qquad \text{and} \qquad \epsilon = \frac{E}{\hbar\omega} \qquad \ldots(7).$$

As ussual, one expects solutions of Eq. (6) to show rapid decline as $z \to \pm\infty$. Our inspection of the asymptotic form, i.e. $z^2 \gg \epsilon$, show $u \sim \exp(-z^2/2)$ is a solution in this region. This therefore suggest general solutions of the form $F(z)\exp(-z^2/2)$, where F is a polynomial. Substituting this form into Eq. (6) yields

$$\frac{d^2F}{dz^2} - 2z\frac{dF}{dz} + (2\epsilon - 1)F = 0 \qquad \ldots(8).$$

Suppose the leading term of F is z^n. This contributes

$$n(n-1)z^{n-2} - 2nz^n + (2\epsilon - 1)z^n \qquad \ldots(9).$$

to the left-hand side of Eq. (8). The coefficient of z^n must vanish to comply with Eq. (8) and as lower-order terms in the polynomial F only contribute to z^{n-1}, or lower powers, we demand from Eq. (9) that

$$\epsilon = n + \frac{1}{2} \qquad n = 1, 2, 3, \ldots \qquad \ldots(10).$$

It follows from Eq. (7) that the energy E is restricted to discrete levels given by

$$E_n = (n + \frac{1}{2})\hbar\omega \qquad \ldots(11).$$

These levels have the interesting property that they are equispaced and the classical frequency ω is related to E in the same way as the photon relation, $E = h\nu$. This is no coincidence.

We have showed that the energy of quantum oscillator is quantized. The ground state, however, has energy $\frac{1}{2}\hbar\omega$ which, as in previous example, is above the classical minimum ($E = 0$). The ground state wave function u_0 is given by $n = 0$ in which case F is constant, so $u_0 \propto \exp(-z^2/2)$. Applying the normalization condition gives a gaussian function

$$u_0 = (m\omega/\pi\hbar)^{1/4}\exp(-m\omega q^2/2\hbar) \qquad \ldots(12).$$

The expectation values of q and V for the ground state are

$$\langle q\rangle = \int_{-\infty}^{\infty} P_0(q) q\, dq = \int_{-\infty}^{\infty} u_0^2 q\, dq = 0 \qquad \ldots(13).$$

$$\langle V\rangle = \frac{k}{2}\int_{-\infty}^{\infty} P_0(q) q^2\, dq = \frac{k}{2}\int_{-\infty}^{\infty} u_0^2 q^2\, dq = \frac{1}{2}E_0 \qquad \ldots(14).$$

respectively

2.2 Further disscusion on quantization

We can see that the Hamiltonian formulation in Eq. (1) take the form of the left-hand side of Eq. (4) by cancelled the $u(q)$ and inserting $V = \frac{1}{2}kq^2$. By putting the wave function ψ instead of $u(q)$ and write E as $i\hbar\frac{\partial}{\partial t}$ we have the Schrödinger equation in the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dq^2}+\frac{1}{2}m\omega^2q^2\psi=i\hbar\frac{\partial\psi}{\partial t} \qquad \ldots(15).$$

By scalling the oscillator by introducing $s=q/q_0$ and $q_0^2=\hbar/m\omega$ yields the Schrödinger equation in terms of s for the wave function $\psi(s,t)$

$$i\hbar\frac{\partial\psi}{\partial t}=\hbar\omega(-\frac{1}{2}\frac{\partial^2\psi}{\partial s^2}+\frac{1}{2}s^2\psi) \qquad \ldots(16).$$

The $\hbar$ may now be cancelled remaining only one parameter ω to define the oscillator. This scalling allow us to find the eigenfunctions for stationary states which satisfy

$$E\psi=\hbar\omega(-\frac{1}{2}\frac{\partial^2\psi}{\partial s^2}+\frac{1}{2}s^2\psi) \qquad \ldots(17).$$

We have already seen that the spectrum is discrete (Eq. (11)), and that the first few eigenfuctions all contain a factor $\exp(-\frac{1}{2}s^2)$ and the other factor being a polynomial. We can setting

$$\psi=f(s)\exp(-\frac{1}{2}s^2) \qquad \ldots(18).$$

by differentiation we have

$$\psi''=(f''-2sf'+(s^2-1)f)\exp(-\frac{1}{2}s^2) \qquad \ldots(19).$$

Inserting in the original equation now gives the equation for f,

$$Ef=\hbar\omega(-\frac{1}{2}f''+sf'+\frac{1}{2}f) \qquad \ldots(20).$$

We may now solve the problem using the power series approach. We see that none of terms is singular for any value for s, so we may expand f as a Taylor series which convergent for all s,

$$f(s) = \sum_{j=0}^{\infty} c_j s^j \qquad \ldots (21).$$

Substitute in the equation and collecting powers of s^j in the result gives

$$Ec_j = \hbar\omega\{-\frac{1}{2}(j+2)(j+1)c_{j+2} + sc_j + \frac{1}{2}c_j\} \qquad \text{for} j \geq 0 \qquad \ldots (22).$$

that is,

$$\frac{1}{2}\hbar\omega(j+2)(j+1)c_{j+2} = \{(j+\frac{1}{2})\hbar\omega - E\}c_j \qquad (j \geq 0) \qquad \ldots (23).$$

We see that if we know c_0 and c_1, any subsequaent coefficient may be obtained by applying this relation a sufficient number of times. It remains ensure that $\psi(s) \to 0$ as $|s| \to \infty$.

Now we have for large j

$$\frac{c_{j+2}}{c_j} = \frac{2}{j} + 0(\frac{1}{j^2}) \qquad \ldots (24).$$

we can see that the coefficients show a behaviour similar to those in the Taylor series of exp s^2. Consequently, $\psi(\equiv f \exp(-\frac{1}{2}s^2))$ is inevitably unbounded as s goes to infinity in either direction, and this will not do. The series for f must therefore terminate and this happens only if

$$E = E_n \equiv (n+\frac{1}{2})\hbar\omega \qquad (n \,\text{interger} \geq 0) \qquad \ldots (25).$$

when the final term in series will be $c_n s^n$. We can compute first few unnormalized function including their time dependence as given bellow,

$$\psi_0 = \exp(-\frac{1}{2}s^2)\exp(-\frac{1}{2}i\omega t).$$
$$\psi_1 = s\exp(-\frac{1}{2}s^2)\exp(-\frac{3}{2}i\omega t).$$
$$\psi_2 = (2s^2-1)\exp(-\frac{1}{2}s^2)\exp(-\frac{5}{2}i\omega t) \qquad \ldots(26).$$

respectively

2.3 The algebraic formulation of the simple harmonic oscilator

We shall carry out the solution of the simple harmonic oscillator using an algebraic formalism based on the Dirac notation. The starting point is the fact that the Hamiltonian is almost factorizable as the difference of two squares,

$$(s-\frac{d}{ds})(s+\frac{d}{ds})\psi(s) = (s^2-\frac{d^2}{ds^2}-1)\psi(s) \qquad \ldots(27).$$

We shall introduce the s-representation by writing $\psi(s) = \langle s|\psi\rangle$ and define two operators a, a^+ by the relations

$$\langle s|\mathsf{a} = 2^{-1/2}(s+\frac{d}{ds})\langle s| \qquad \ldots(28).$$

$$\langle s|\mathsf{a}^+ = 2^{-1/2}(s-\frac{d}{ds})\langle s| \qquad \ldots(29).$$

Then

$$\hbar\omega\langle s|\mathsf{a}^{+}\mathsf{a} = \frac{\hbar\omega}{2}(s + \frac{d}{ds})(s - \frac{d}{ds})\langle s| = \langle s|(\mathsf{H} - \frac{1}{2}\hbar\omega) \qquad \ldots(30).$$

whence

$$\mathsf{H} = \hbar\omega(\mathsf{a}^{+}\mathsf{a} + \frac{1}{2}) = \hbar\omega(n + \frac{1}{2}) \qquad \ldots(31).$$

which show us about the quantization on the energy of the oscillator.

2.4 The Wilson-Sommerfeld rules of quantization

This rules discovered by W. Wilson and A. Sommerfeld independently in 1915[7]. This method consists in solving the classical equation of motion in the Hamiltonian form, therefore applying the coordinates $q_1, \ldots, q_{3n}$ and the canonically conjugate momenta $p_1, \ldots, p_{3n}$ as the independent variables. The assumption is the introduced that only those classical orbits are allowed as stasionary states for which the following condition are satisfied,

$$\oint p_k\, dq_k = n_k h, \qquad k = 1, 2, \ldots, 3n \qquad n_k = \text{an integer} \qquad \ldots(32).$$

This integrals can be calculated only for conditionally periodic systems, i.e. for systems for which coordinates can be found each of which goes through a cycle as a function of the time, independently of the others. Sometimes the coordinates can be chosen in several different ways, in which case the shapes of the quantized orbits depend on the choice of coordinate systems, but the energy values do not.

3 Concluding Remark

It follows from Eq. (14) and the followed description that the expectation value of the kinetic energy $\langle E_0\rangle - \langle V\rangle$ is $\frac{1}{2}E_0$ also. As in the classical case,

the average kinetic and potential energies are the same. This remains true for the excited levels ($n \geq 1$). We could construct such levels wave function by substitute a full polynomial for F in Eq. (8) and equate the coefficients of all the powers (not just z^n) to zero.

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